10558931.trn

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1626GMS

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	MAY 01	New CAS web site launched
NEWS 3	MAY 08	CA/CAplus Indian patent publication number format defined
NEWS 4	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 5	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS 6	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS 7	MAY 21	CA/CAplus enhanced with additional kind codes for German patents
NEWS 8	MAY 22	CA/CAplus enhanced with IPC reclassification in Japanese patents
NEWS 9	JUN 27	CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 10	JUN 29	STN Viewer now available
NEWS 11	JUN 29	STN Express, Version 8.2, now available
NEWS 12	JUL 02	LEMBASE coverage updated
NEWS 13	JUL 02	LMEDLINE coverage updated
NEWS 14	JUL 02	SCISEARCH enhanced with complete author names
NEWS 15	JUL 02	CHEMCATS accession numbers revised
NEWS 16	JUL 02	CA/CAplus enhanced with utility model patents from China
NEWS 17	JUL 16	CAplus enhanced with French and German abstracts
NEWS 18	JUL 18	CA/CAplus patent coverage enhanced
NEWS 19	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 20	JUL 30	USGENE now available on STN
NEWS 21	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 22	AUG 06	BEILSTEIN updated with new compounds
NEWS 23	AUG 06	FSTA enhanced with new thesaurus edition

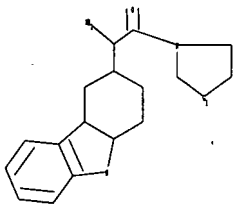
NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

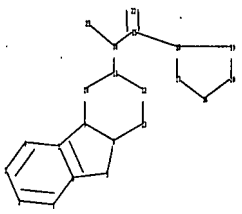
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

```
* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:18:22 ON 10 AUG 2007

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files.  For example, the EXPAND
command can only be used to look at the index in a file which has an
index.  Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 14:18:31 ON 10 AUG 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:     9 AUG 2007  HIGHEST RN 944380-35-2
DICTIONARY FILE UPDATES:    9 AUG 2007  HIGHEST RN 944380-35-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10558931.str
```





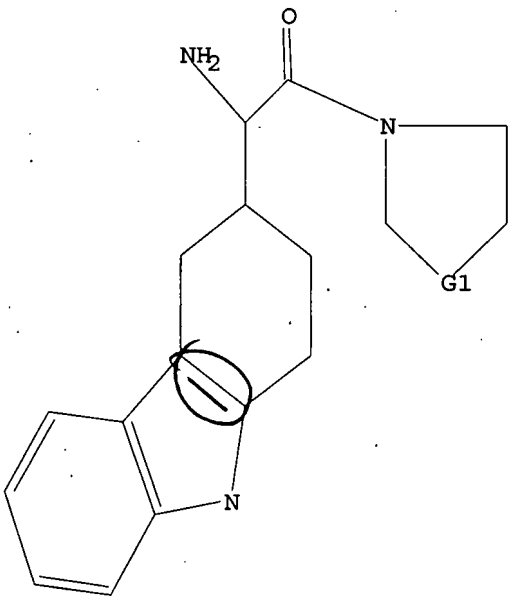
chain nodes :
14 15 22 23
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 16 17 18 19 20
chain bonds :
11-14 14-15 14-23 15-18 15-22
ring bonds :
1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13
16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
5-8 5-6 7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15 14-23 15-18
15-22 16-17 16-20 17-18 18-19 19-20
normalized bonds :
1-2 1-6 2-3 3-4 4-7 6-7
isolated ring systems :
containing 1 : 16 :

G1:S,CH2,CH,CF2,SO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 22:CLASS 23:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 14:18:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 0 TO 0
PROJECTED ANSWERS: 0 TO 0

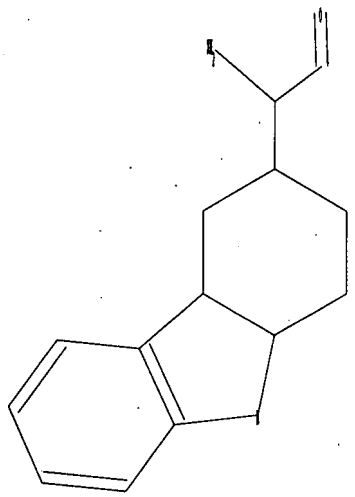
L2 0 SEA SSS SAM L1

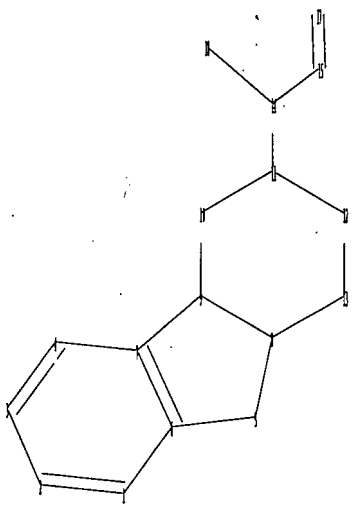
=> s l1 sss full
FULL SEARCH INITIATED 14:18:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 52 TO ITERATE

100.0% PROCESSED 52 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=>
Uploading C:\Program Files\Stnexp\Queries\10558931a.str





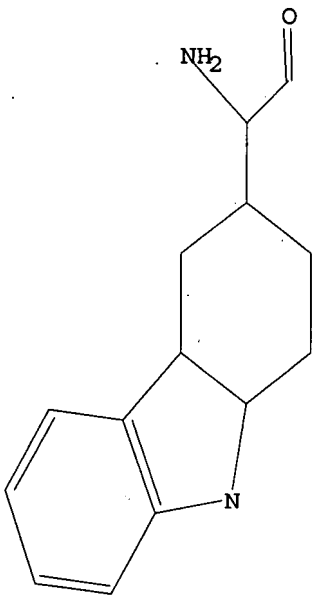
chain nodes :
14 15 17 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
11-14 14-15 14-18 15-17
ring bonds :
1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13
exact/norm bonds :
5-8 5-6 14-18 15-17
exact bonds :
7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15
normalized bonds :
1-2 1-6 2-3 3-4 4-7 6-7
isolated ring systems :
containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 17:CLASS 18:CLASS

L4 STRUCTURE UPLOADED

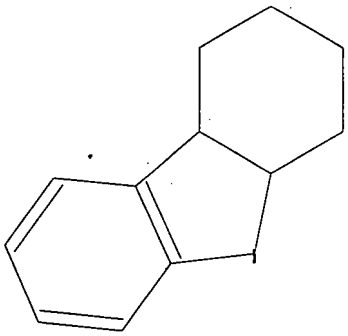
=> d l4
L4 HAS NO ANSWERS
L4 STR

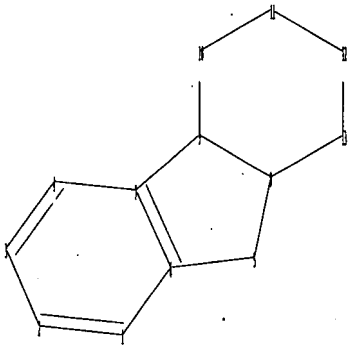


G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

```
=> s l4
SAMPLE SEARCH INITIATED 14:20:09 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       39 TO ITERATE

100.0% PROCESSED       39 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          406 TO     1154
PROJECTED ANSWERS:               0 TO        0

L5             0 SEA SSS SAM L4

=> s l4 sss full
FULL SEARCH INITIATED 14:20:15 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      740 TO ITERATE

100.0% PROCESSED      740 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L6             0 SEA SSS FUL L4

=>
Uploading C:\Program Files\Stnexp\Queries\10558931b.str
```





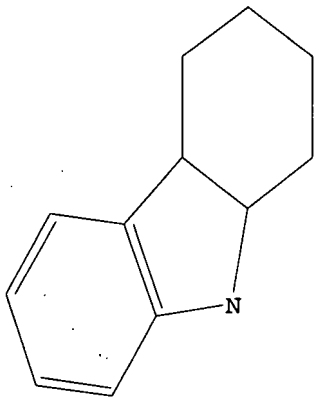
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
ring bonds :
1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13
exact/norm bonds :
5-8 5-6
exact bonds :
7-9 8-13 8-9 9-10 10-11 11-12 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-7 6-7
isolated ring systems :
containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom

L7 STRUCTURE UPLOADED

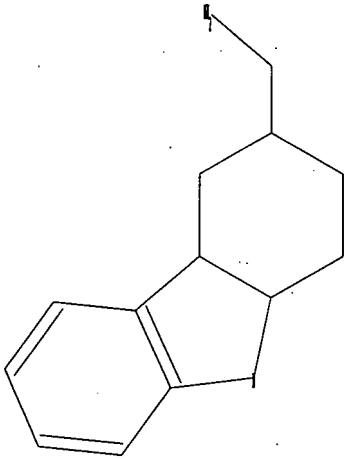
=> d l7
L7 HAS NO ANSWERS
L7 STR

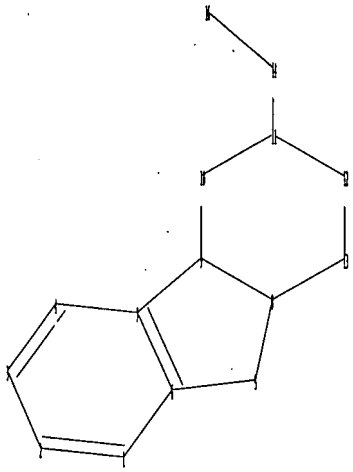


G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

```
=> s l7
SAMPLE SEARCH INITIATED 14:21:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     2011 TO ITERATE

 99.5% PROCESSED     2000 ITERATIONS                                 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        37530 TO    42910
PROJECTED ANSWERS:             740 TO     1672

L8            50 SEA SSS SAM L7

=> s l7 sss full
FULL SEARCH INITIATED 14:21:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    38933 TO ITERATE

100.0% PROCESSED    38933 ITERATIONS                               1220 ANSWERS
SEARCH TIME: 00.00.01

L9          1220 SEA SSS FUL L7

=>
Uploading C:\Program Files\Stnexp\Queries\10558931c.str
```





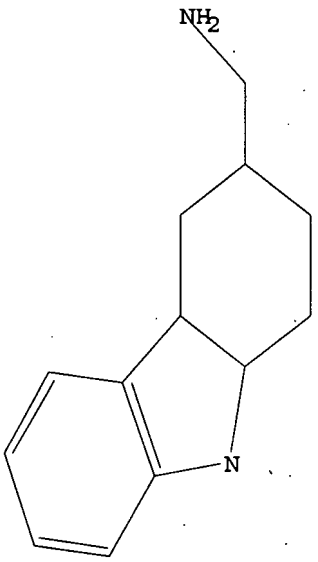
chain nodes :
14 16
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
11-14 14-16
ring bonds :
1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13
exact/norm bonds :
5-8 5-6 14-16
exact bonds :
7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-7 6-7
isolated ring systems :
containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 16:CLASS

L10 STRUCTURE UPLOADED

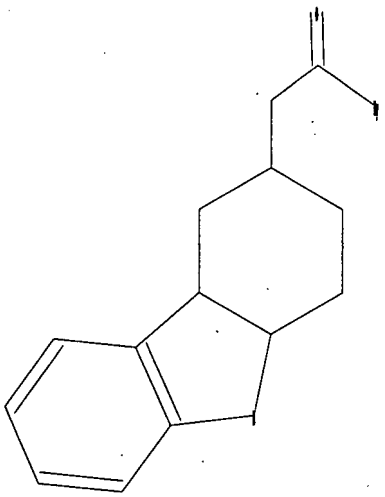
=> d l10
L10 HAS NO ANSWERS
L10 STR

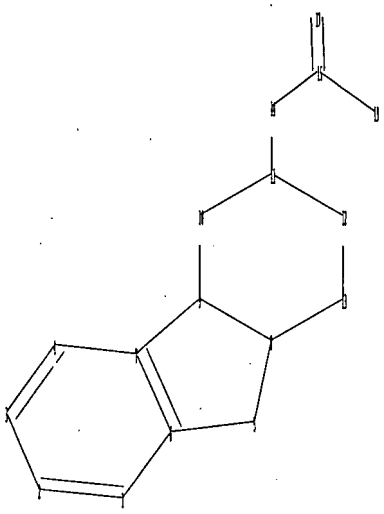


G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

```
=> s l10
SAMPLE SEARCH INITIATED 14:22:55 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      216 TO ITERATE

100.0% PROCESSED      216 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         3439 TO     5201
PROJECTED ANSWERS:               0 TO        0

L11           0 SEA SSS SAM L10

=> s l10 sss full
FULL SEARCH INITIATED 14:23:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     3888 TO ITERATE

100.0% PROCESSED     3888 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L12           0 SEA SSS FUL L10

=>
Uploading C:\Program Files\Stnexp\Queries\10558931d.str
```





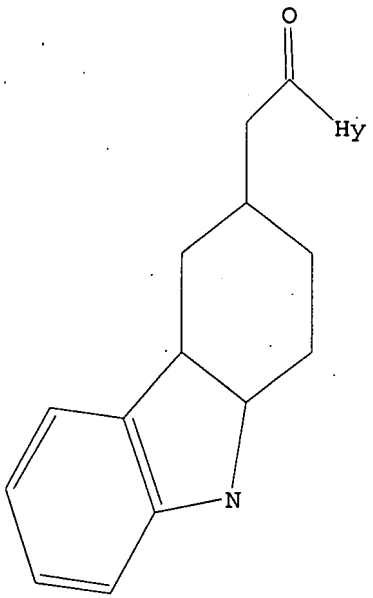
chain nodes :
14 15 17 19
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
11-14 14-15 15-17 15-19
ring bonds :
1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13
exact/norm bonds :
5-8 5-6 15-17 15-19
exact bonds :
7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15
normalized bonds :
1-2 1-6 2-3 3-4 4-7 6-7
isolated ring systems :
containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 17:CLASS 19:CLASS

L13 STRUCTURE UPLOADED

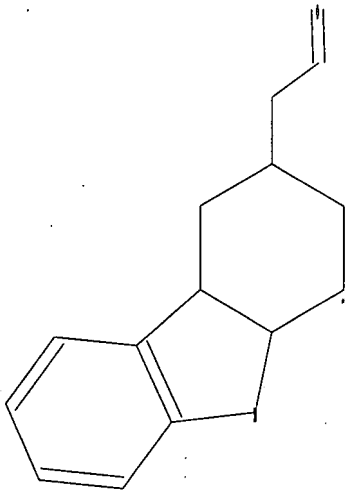
=> d l13
L13 HAS NO ANSWERS
L13 STR

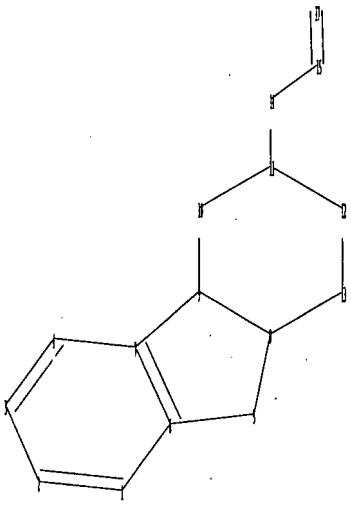


G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

```
=> s l13
SAMPLE SEARCH INITIATED 14:24:43 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       244 TO ITERATE

100.0% PROCESSED      244 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         3943 TO     5817
PROJECTED ANSWERS:               0 TO        0

L14            0 SEA SSS SAM L13

=> s l13 sss full
FULL SEARCH INITIATED 14:24:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     4979 TO ITERATE

100.0% PROCESSED     4979 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

L15            0 SEA SSS FUL L13

=>
Uploading C:\Program Files\Stnexp\Queries\10558931e.str
```





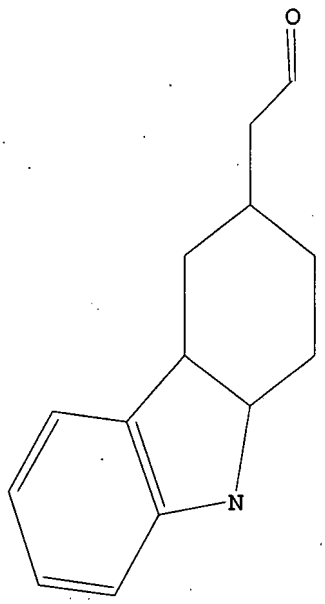
chain nodes :
14 15 17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
11-14 14-15 15-17
ring bonds :
1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13
exact/norm bonds :
5-8 5-6 15-17
exact bonds :
7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15
normalized bonds :
1-2 1-6 2-3 3-4 4-7 6-7
isolated ring systems :
containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 17:CLASS

L16 STRUCTURE UPLOADED

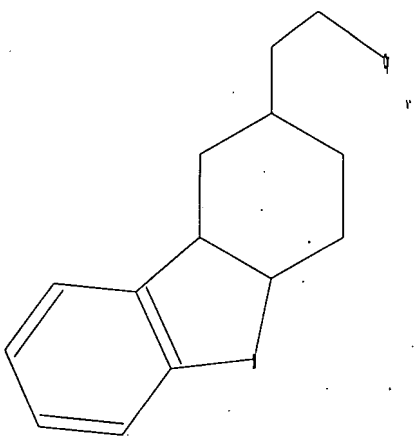
=> d l16
L16 HAS NO ANSWERS
L16 STR

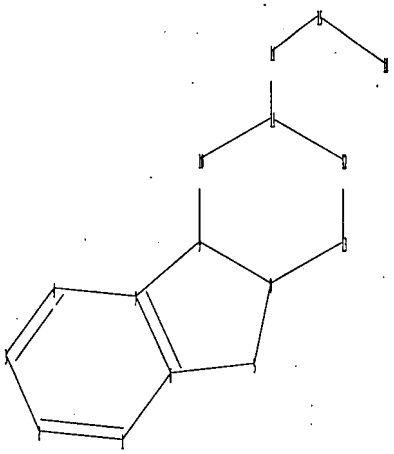


G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

```
=> s l16
SAMPLE SEARCH INITIATED 14:27:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       244 TO ITERATE

100.0% PROCESSED      244 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          3943 TO     5817
PROJECTED ANSWERS:                0 TO        0

L17            0 SEA SSS SAM L16

=> s l16 sss full
FULL SEARCH INITIATED 14:27:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     4979 TO ITERATE

100.0% PROCESSED     4979 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L18            0 SEA SSS FUL L16

=>
Uploading C:\Program Files\Stnexp\Queries\10558931f.str
```





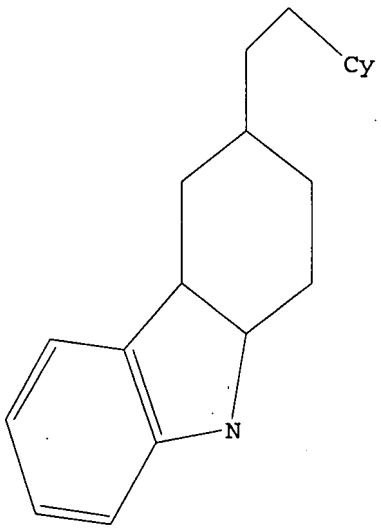
chain nodes :
14 15 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
11-14 14-15 15-18
ring bonds :
1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13
exact/norm bonds :
5-8 5-6 15-18
exact bonds :
7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15
normalized bonds :
1-2 1-6 2-3 3-4 4-7 6-7
isolated ring systems :
containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 18:CLASS

L19 STRUCTURE UPLOADED

=> d l19
L19 HAS NO ANSWERS
L19 STR

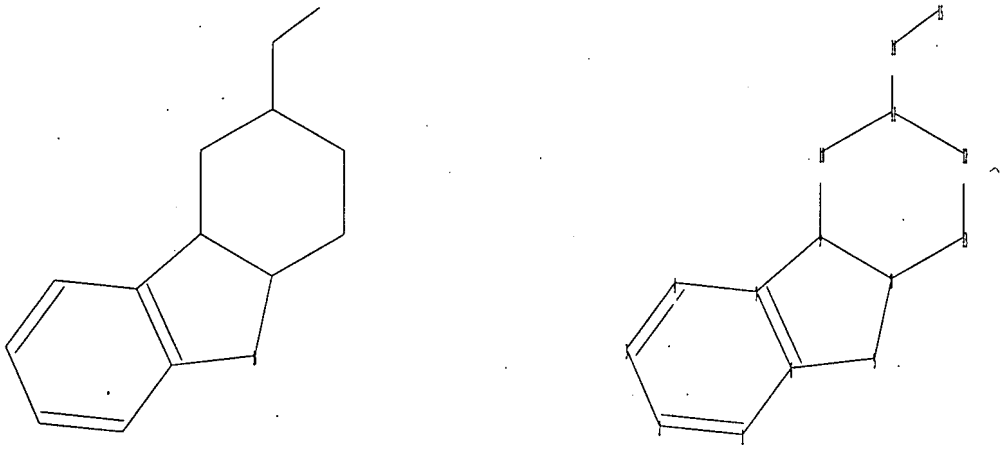


G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

```
=> s l19
SAMPLE SEARCH INITIATED 14:30:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      954 TO ITERATE

100.0% PROCESSED      954 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        17227 TO    20933
PROJECTED ANSWERS:               0 TO        0

L20           0 SEA SSS SAM L19

=> s l19 sss full
FULL SEARCH INITIATED 14:30:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    17864 TO ITERATE

100.0% PROCESSED    17864 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L21           0 SEA SSS FUL L19

=> d his

     (FILE 'HOME' ENTERED AT 14:18:22 ON 10 AUG 2007)

     FILE 'REGISTRY' ENTERED AT 14:18:31 ON 10 AUG 2007
L1              STRUCTURE UPLOADED
L2            0 S L1
L3            0 S L1 SSS FULL
L4              STRUCTURE UPLOADED
L5            0 S L4
```

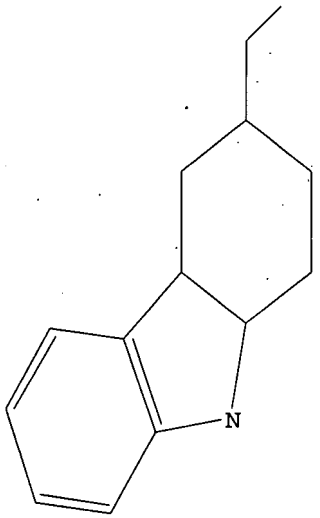
```
L6             0 S L4 SSS FULL
L7               STRUCTURE UPLOADED
L8            50 S L7
L9          1220 S L7 SSS FULL
L10              STRUCTURE UPLOADED
L11            0 S L10
L12            0 S L10 SSS FULL
L13              STRUCTURE UPLOADED
L14            0 S L13
L15            0 S L13 SSS FULL
L16              STRUCTURE UPLOADED
L17            0 S L16
L18            0 S L16 SSS FULL
L19              STRUCTURE UPLOADED
L20            0 S L19
L21            0 S L19 SSS FULL

=>
Uploading C:\Program Files\Stnexp\Queries\10558931g.str
```



```
chain nodes :
14  15
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13
chain bonds :
11-14  14-15
ring bonds :
1-2  1-6  2-3  3-4  4-7  5-8  5-6  6-7  7-9  8-13  8-9  9-10  10-11  11-12  12-13
exact/norm bonds :
5-8  5-6
exact bonds :
7-9  8-13  8-9  9-10  10-11  11-12  11-14  12-13  14-15
normalized bonds :
1-2  1-6  2-3  3-4  4-7  6-7
isolated ring systems :
containing 1 :


G1:S,CH2,CH,CF2,SO2

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:CLASS  15:CLASS
```

L22 STRUCTURE UPLOADED

=> d l22
L22 HAS NO ANSWERS
L22 STR



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l22
SAMPLE SEARCH INITIATED 14:32:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1082 TO ITERATE

100.0% PROCESSED 1082 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 19667 TO 23613
PROJECTED ANSWERS: 2 TO 124

L23 2 SEA SSS SAM L22

=> s l22 sss full
FULL SEARCH INITIATED 14:32:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 20417 TO ITERATE

100.0% PROCESSED 20417 ITERATIONS 36 ANSWERS
SEARCH TIME: 00.00.01

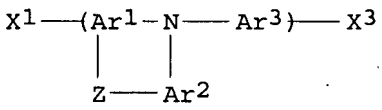
L24 36 SEA SSS FUL L22

=> d his

```
     (FILE 'HOME' ENTERED AT 14:18:22 ON 10 AUG 2007)

     FILE 'REGISTRY' ENTERED AT 14:18:31 ON 10 AUG 2007
L1                STRUCTURE UPLOADED
L2              0 S L1
L3              0 S L1 SSS FULL
L4                STRUCTURE UPLOADED
L5              0 S L4
L6              0 S L4 SSS FULL
L7                STRUCTURE UPLOADED
L8             50 S L7
L9           1220 S L7 SSS FULL
L10               STRUCTURE UPLOADED
L11             0 S L10
L12             0 S L10 SSS FULL
L13               STRUCTURE UPLOADED
L14             0 S L13
L15             0 S L13 SSS FULL
L16               STRUCTURE UPLOADED
L17             0 S L16
L18             0 S L16 SSS FULL
L19               STRUCTURE UPLOADED
L20             0 S L19
L21             0 S L19 SSS FULL
L22               STRUCTURE UPLOADED
L23             2 S L22
L24            36 S L22 SSS FULL

=> FIL HCAPLUS
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                            1384.00    1384.21

FILE 'HCAPLUS' ENTERED AT 14:33:02 ON 10 AUG 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
the American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 10 Aug 2007  VOL 147 ISS 8
FILE LAST UPDATED: 9 Aug 2007  (20070809/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> s l24
L25          15 L24
```

```
=> s l9
L26         472 L9

=> s l25 and py<=2003
      23927587 PY<=2003
L27          14 L25 AND PY<=2003

=> s l26 and p/dt
        5818845 P/DT
L28         127 L26 AND P/DT

=> s l28 and us/pc
        1705037 US/PC
L29          57 L28 AND US/PC

=> s l29 and py<=2003
      23927587 PY<=2003
L30          51 L29 AND PY<=2003

=> s l30 and dipeptidyl
           4690 DIPEPTIDYL
L31           0 L30 AND DIPEPTIDYL

=> s l30 and thu
            159 THU
        2428717 THUS
        2428858 THU
                  (THU OR THUS)
L32          28 L30 AND THU

=> s l32 and diabetes
         128376 DIABETES
L33           0 L32 AND DIABETES

=> s l32 and disease
         978988 DISEASE
         264275 DISEASES
        1096696 DISEASE
                  (DISEASE OR DISEASES)
L34           4 L32 AND DISEASE

=> d his

     (FILE 'HOME' ENTERED AT 14:18:22 ON 10 AUG 2007)

     FILE 'REGISTRY' ENTERED AT 14:18:31 ON 10 AUG 2007
L1                STRUCTURE UPLOADED
L2              0 S L1
L3              0 S L1 SSS FULL
L4                STRUCTURE UPLOADED
L5              0 S L4
L6              0 S L4 SSS FULL
L7                STRUCTURE UPLOADED
L8             50 S L7
L9           1220 S L7 SSS FULL
L10               STRUCTURE UPLOADED
L11             0 S L10
L12             0 S L10 SSS FULL
L13               STRUCTURE UPLOADED
L14             0 S L13
```

```
L15             0 S L13 SSS FULL
L16               STRUCTURE UPLOADED
L17             0 S L16
L18             0 S L16 SSS FULL
L19               STRUCTURE UPLOADED
L20             0 S L19
L21             0 S L19 SSS FULL
L22               STRUCTURE UPLOADED
L23             2 S L22
L24            36 S L22 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 14:33:02 ON 10 AUG 2007
L25            15 S L24
L26           472 S L9
L27            14 S L25 AND PY<=2003
L28           127 S L26 AND P/DT
L29            57 S L28 AND US/PC
L30            51 S L29 AND PY<=2003
L31             0 S L30 AND DIPEPTIDYL
L32            28 S L30 AND THU
L33             0 S L32 AND DIABETES
L34             4 S L32 AND DISEASE

=> d l25 ibib abs hitstr tot

L25  ANSWER 1 OF 15  HCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2006:656254  HCAPLUS
DOCUMENT NUMBER:          145:125169
TITLE:                    Rigid amines for use in manufacture of conjugated
                          polymer useful as emitters, charge transporters or
                          host materials in opto-electrical devices
INVENTOR(S):              Heidenhain, Sophie; Leadbeater, Mark; Steudel,
                          Annette; Hicks, Daniel
PATENT ASSIGNEE(S):       Cambridge Display Technology Limited, UK; CDT Oxford
                          Limited
SOURCE:                   PCT Int. Appl., 49 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
     WO 2006070185         A1    20060706    WO 2005-GB5058          20051223
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.:                   GB 2004-28443       A  20041229
                                         GB 2005-2254        A  20050203
GI
```



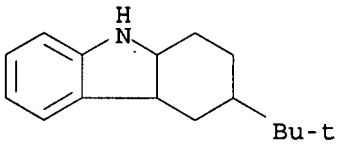
I

AB The monomer has a structure as shown in I where: Ar1, Ar2 and Ar3 are independently selected from optionally substituted aryl or heteroaryl, X1 and X3 both independently comprise a leaving group capable of participating in polymerization and Z represents a direct bond or an optionally substituted bridging atom.

IT 6731-89-1P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(manufacture of rigid amines as monomers for conjugated polymer useful for emitters, charge transporters or host materials in opto-elec. devices)

RN 6731-89-1 HCAPLUS

CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:363554 HCAPLUS

DOCUMENT NUMBER: 131:115858

TITLE: Alkylation of ketone and ester lithium enolates with nitroethylene

AUTHOR(S): Flintoft, Rebecca J.; Buzby, Jennifer C.; Tucker, John A.

CORPORATE SOURCE: Medicinal Chemistry Research, Pharmacia and Upjohn, Kalamazoo, MI, 49001, USA

SOURCE: Tetrahedron Letters (1999), 40(24), 4485-4488
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 131:115858

AB We describe the first systematic study of the scope and limitations of the conjugate addition of ketone and ester enolates to nitroethylene. Synthetically useful yields are obtained for ketone and ester enolates of a variety of structural types.

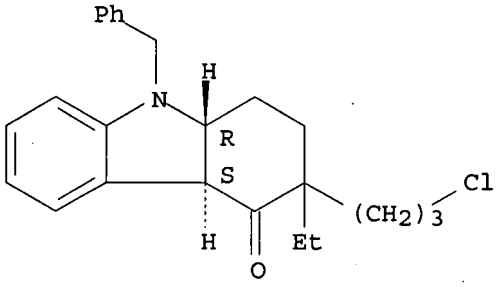
IT 232923-95-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of ketone enolates or ester enolates with nitroethylene)

RN 232923-95-4 HCAPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-

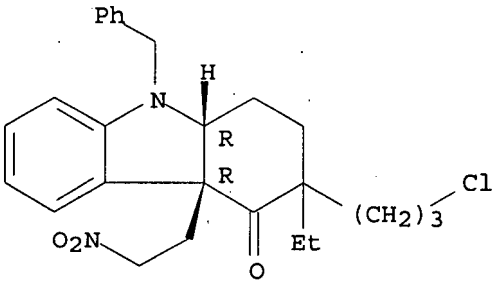
(phenylmethyl)-, (4aR,9aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



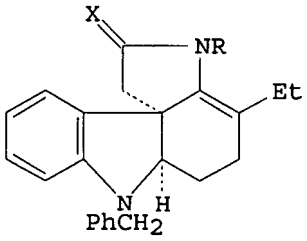
IT 232924-06-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(alkylation of ketone enolates or ester enolates with nitroethylene)
RN 232924-06-0 HCAPLUS
CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (4aR,9aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

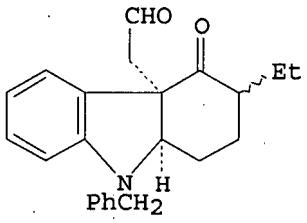


REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

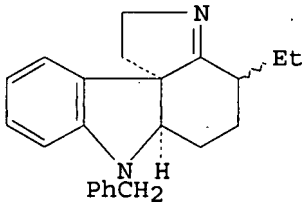
L25 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:631122 HCAPLUS
DOCUMENT NUMBER: 121:231122
TITLE: Unexpected results in the reduction of tetracyclic enamides. Structure, stereochemistry and conformation of a 20β-hydroperoxyimine
AUTHOR(S): Dugat, Denise; Dauphin, Gerard; Gramain, Jean-Claude
CORPORATE SOURCE: Universite Blaise Pascal de Clermont-Ferrand, Aubiere, 63177, Fr.
SOURCE: Heterocycles (1994), 38(8), 1909-18
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



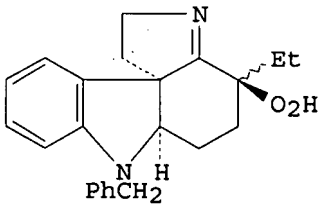
I



II



III



IV

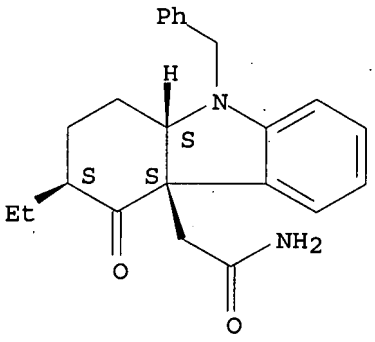
AB Reduction of Nb-allyl-20-ethyltetracyclic enamide I (X = O, R = allyl) with lithium aluminum hydride afforded the expected enamine I (X = H2, R = allyl) and 4a-oxoethylhexahydrocarbazolones II. Reduction of Nb-unsubstituted enamide I (X = O, R = H), under the same conditions, gave imine III, enamine I (X = H2, R = H) and a 20β-hydroperoxytetracyclic imine IV resulting from peroxydation. The C-20 stereochem. of IV was established by means of 2D 1H NMR and NOE difference spectroscopy.

IT 158148-36-8P 158148-37-9P 158148-38-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and intramol. cyclization of)

RN 158148-36-8 HCAPLUS

CN 4aH-Carbazole-4a-acetamide, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3α,4aα,9aα)- (9CI) (CA INDEX NAME)

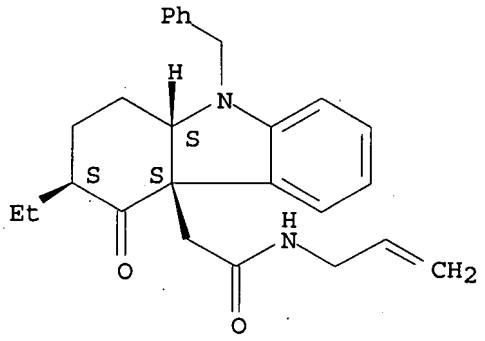
Relative stereochemistry.



RN 158148-37-9 HCAPLUS

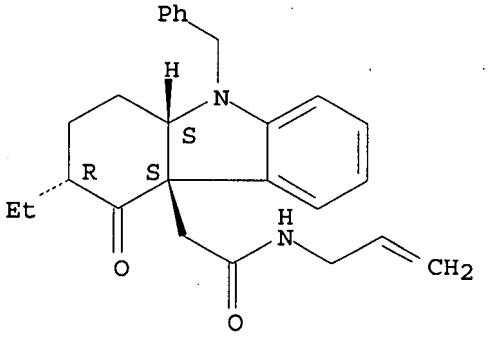
CN 4aH-Carbazole-4a-acetamide, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-N-2-propenyl-, (3α,4aα,9aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



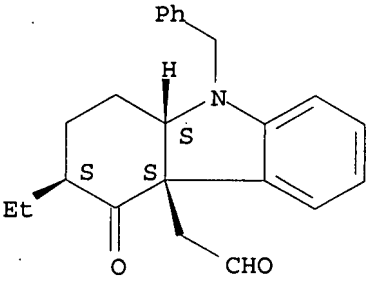
RN 158148-38-0 HCAPLUS
CN 4aH-Carbazole-4a-acetamide, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-N-2-propenyl-, (3α,4aβ,9aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



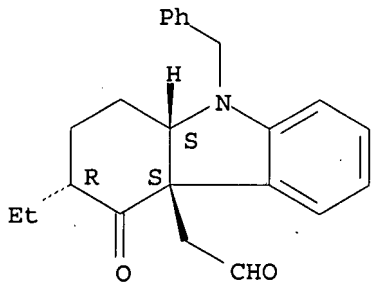
IT 158148-44-8P 158148-45-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 158148-44-8 HCAPLUS
CN 4aH-Carbazole-4a-acetaldehyde, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3α,4aα,9aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



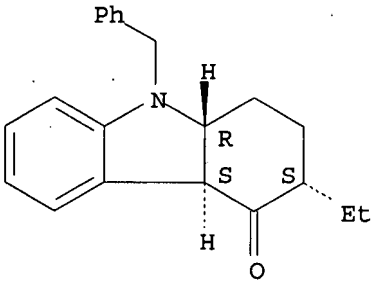
RN 158148-45-9 HCAPLUS
CN 4aH-Carbazole-4a-acetaldehyde, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3α,4aβ,9aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



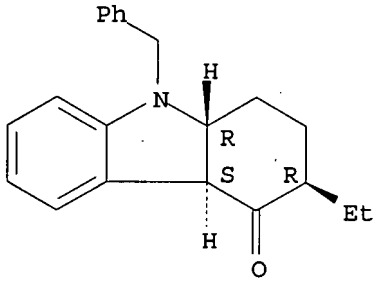
IT 129574-42-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with iodoacetamide)
RN 129574-42-1 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3α,4aα,9aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 129574-41-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with iodoacetamides)
RN 129574-41-0 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3α,4aβ,9aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



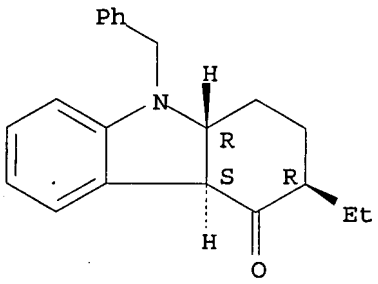
L25 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:134890 HCAPLUS

DOCUMENT NUMBER: 120:134890
TITLE: Stereocontrolled formation of octahydro-1H-pyrrolo[2,3-d]carbazoles by reductive cyclization: total synthesis of (±)-N-benzylaspidospermidine
AUTHOR(S): Benchekroun-Mounir, Nora; Dugat, Denise; Gramain, Jean Claude; Husson, Henri Philippe
CORPORATE SOURCE: URA, Univ. Blaise Pascal Clermont-Ferrand, Aubiere, 63177, Fr.
SOURCE: Journal of Organic Chemistry (1993), 58(23), 6457-65
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:134890
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

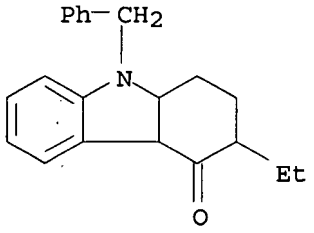
AB The synthesis of a series of 20-substituted octahydro-1H-pyrrolo[2,3-d]carbazoles, intermediates in the synthesis of Aspidosperma alkaloids, is described. Nonoxidative photocyclization of aryl enaminone I led to hexahydrocarbazol-4-ones II. Alkylation of the anions derived from II with KH and iodoacetonitrile gave rise to an undesirable intramol. cyclization while reaction with LDA and nitroethylene as Michael acceptor afforded the trisubstituted hexahydrocarbazolones III (R = CH2CH2CH2Cl). Reductive cyclization (H2,PtO2) of cyano model compds. provided octahydro-1H-pyrrolo[2,3-d]carbazoles whose stereochem. depended on hindrance of the α and β face of the mol. In contrast, reduction (HCOONH4, Pd/C, and then Na/EtOH) of nitro model compds. III (R = H) via nitrones led essentially to the more stable isomers IV with the natural stereochem. at C-21. Reduction (HCOONH4, Pd/C) of nitro compds. III (R = CH2CH2CH2Cl), which possess the elements for the future construction of the D and E rings, induced a tandem cyclization and afforded the pentacyclic iminium which was converted by catalytic hydrogenation into (±)-N-benzylaspidospermidine (V). This compound was thus synthesized in seven steps from N-benzylaniline and cyclohexane-1,3-dione.
IT 129574-41-0 129574-43-2
RL: PROC (Process)
(addition of, with nitroethylene)
RN 129574-41-0 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3α,4aβ,9aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



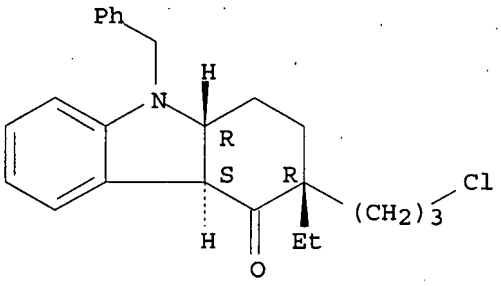
RN 129574-43-2 HCAPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3α,4aα,9aα)- (9CI) (CA INDEX NAME)



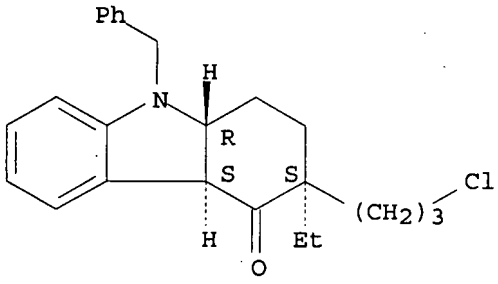
IT 143466-44-8P 143466-49-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and addition of, with nitroethylene)
RN 143466-44-8 HCAPLUS
CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3α,4aα,9aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 143466-49-3 HCAPLUS
CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3α,4aβ,9aα)- (9CI) (CA INDEX NAME)

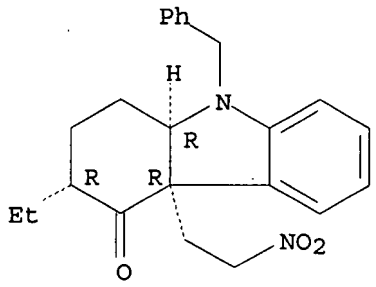
Relative stereochemistry.



IT 152710-80-0P 152710-81-1P 152710-89-9P
152710-90-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 152710-80-0 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-

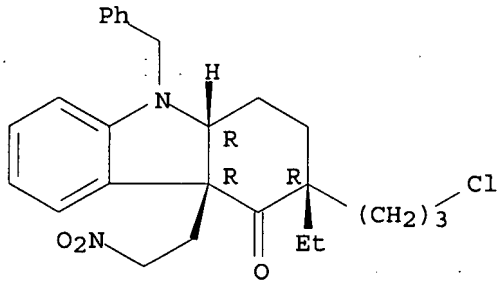
(phenylmethyl)-, (3α,4aα,9aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



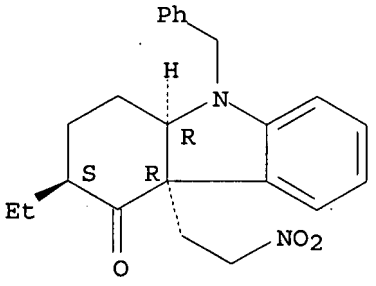
RN 152710-81-1 HCAPLUS
CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3α,4aβ,9aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



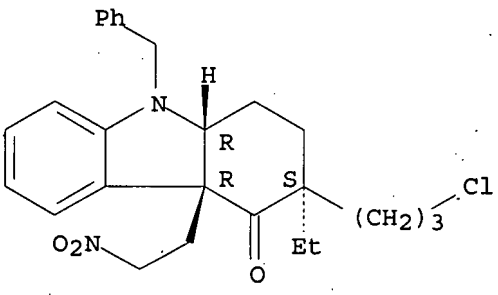
RN 152710-89-9 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3α,4aβ,9aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



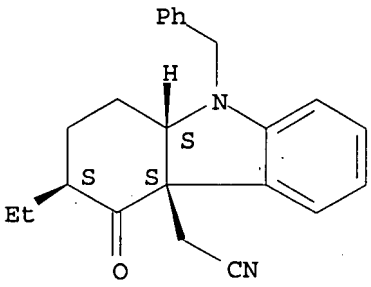
RN 152710-90-2 HCAPLUS
CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3α,4aα,9aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



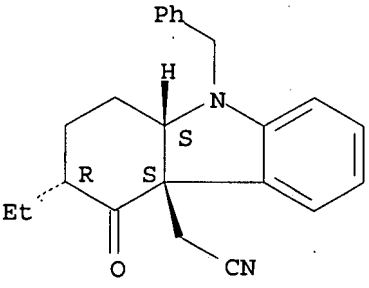
IT 152710-78-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive intramol. cyclization of)
RN 152710-78-6 HCAPLUS
CN 4aH-Carbazole-4a-acetonitrile, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3α,4aα,9aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



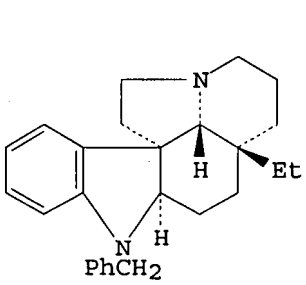
IT 152710-88-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 152710-88-8 HCAPLUS
CN 4aH-Carbazole-4a-acetonitrile, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3α,4aβ,9aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

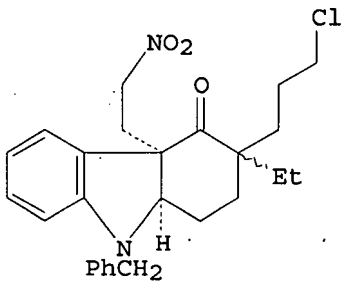


L25 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:571783 HCAPLUS
DOCUMENT NUMBER: 117:171783
TITLE: A short synthesis of (±)-N-benzyl aspidospermidine

AUTHOR(S): Benchekroun-Mounir, Nora; Dugat, Denise; Gramain, Jean Claude
CORPORATE SOURCE: Univ. Blaise Pascal de Clemont-Ferrand, Aubiere, 63177, Fr.
SOURCE: Tetrahedron Letters (1992), 33(28), 4001-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:171783
GI



I



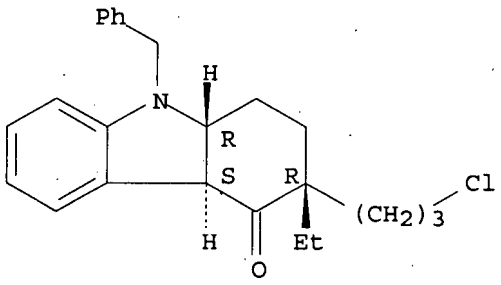
II

AB (±)-N-Benzyl aspidospermidine (I) is synthesized in seven steps via the trisubstituted hexahydrocarbazolone II; reductive cyclization of this intermediate which is obtained by photocyclization and Michael reaction with nitroethylene, creates simultaneously both E and D rings of the pentacyclic system.

IT 143466-44-8P 143466-49-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alkylation of, with nitroethylene)

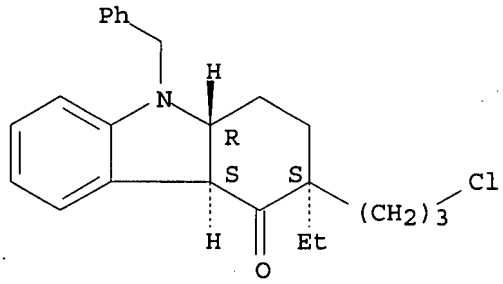
RN 143466-44-8 HCAPLUS
CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3α,4aα,9aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



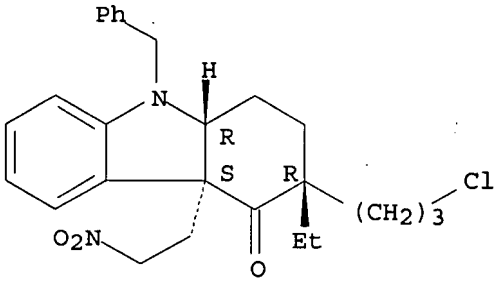
RN 143466-49-3 HCAPLUS
CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3α,4aβ,9aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



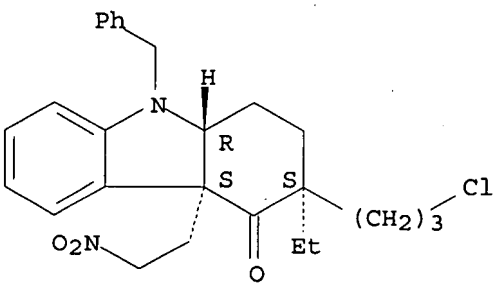
IT 143466-45-9P 143466-48-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive cyclization of)
RN 143466-45-9 HCAPLUS
CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3α,4aα,9aβ)- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



RN 143466-48-2 HCAPLUS
CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3α,4aβ,9aα)- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



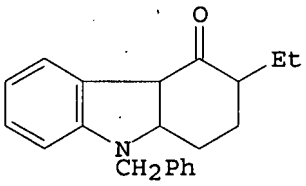
L25 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:552186 HCAPLUS
DOCUMENT NUMBER: 113:152186
TITLE: Structure, stereochemistry, and conformation of

diastereoisomeric cis- and trans-3-ethyl-1,2,3,4,4a,9a-hexahydrocarbazol-4-ones by means of 13C and two-dimensional proton NMR spectroscopy. An example of diastereoselection in a photocyclization reaction

AUTHOR(S): Dugat, Denise; Gramain, Jean Claude; Dauphin, Gerard
CORPORATE SOURCE: Unite Rech., Univ. Blaise Pascal Clermont-Ferrand, Aubiere, 63177, Fr.

SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1990), (4), 605-11
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:152186

GI



I

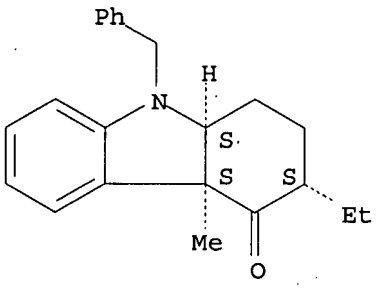
AB Diastereoisomers of 3-ethylhexahydrocarbazol-4-one (I) are stereospecifically obtained in a 4a,9a-trans-configuration by a photocyclization reaction in which appreciable diastereoselection (40%) due to the Et chain is observed They are quant. converted to cis compds. by treatment with acid or by angular alkylation via a benzylic carbanion. Complete anal. of the 1H (1D, 2D) NMR spectra allows the conformation of the C ring in each compound to be established. Moreover, the collected 1H and 13C NMR data constitute refs. for further identification of the cis and trans series and further determination of the position of the 3-Et chain. Equilibrium studies between the different isomers show the higher stability of the cis derivs. which possess the configuration of the natural products of the Aspidosperma indole alkaloids.

IT 129574-45-4 129574-46-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(NMR of carbon-13 and hydrogen in)

RN 129574-45-4 HCAPLUS

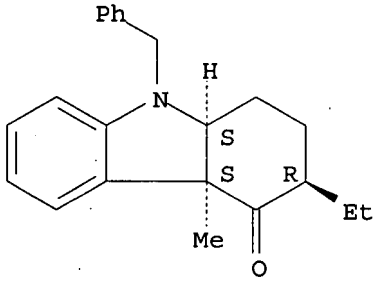
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-methyl-9-(phenylmethyl)-, (3α,4aα,9aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



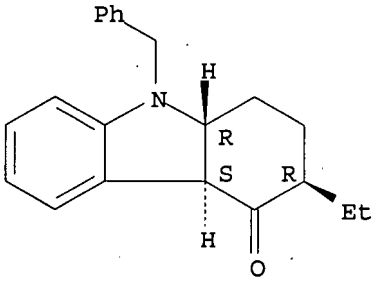
RN 129574-46-5 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-methyl-9-(phenylmethyl)-, (3α,4aβ,9aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



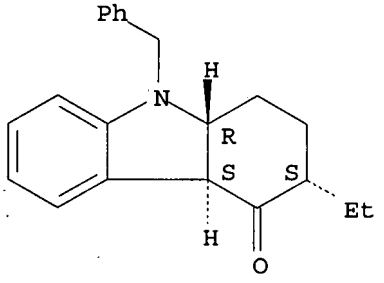
IT 129574-41-0P 129574-42-1P 129574-43-2P
129574-44-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR of)
RN 129574-41-0 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3α,4aβ,9aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



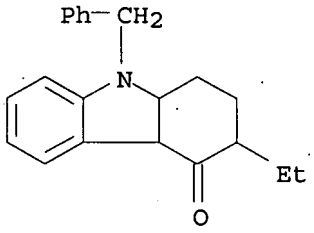
RN 129574-42-1 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3α,4aα,9aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



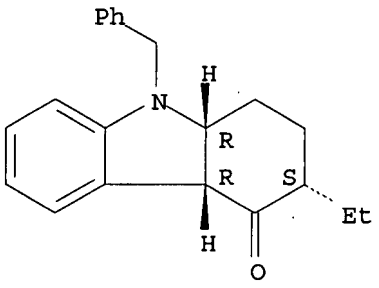
RN 129574-43-2 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-,

(3α,4aα,9aα)- (9CI) (CA INDEX NAME)

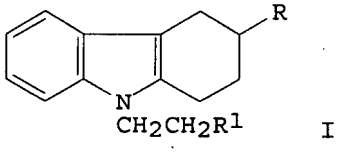


RN 129574-44-3 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3α,4aβ,9aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1987:67041 HCAPLUS
DOCUMENT NUMBER: 106:67041
TITLE: Tetrahydrocarbazoles. Part II. Tricyclic inhibitors of gastric acid secretion
AUTHOR(S): Canas-Rodriguez, A.; Mateo Bernardo, A.
CORPORATE SOURCE: Chelsea Coll., Univ. London, London, SW3 6LX, UK
SOURCE: Anales de Quimica, Serie C: Quimica Organica y Bioquimica (1985), 81(3), 254-7
CODEN: AQSBD6; ISSN: 0211-1357
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:67041
GI

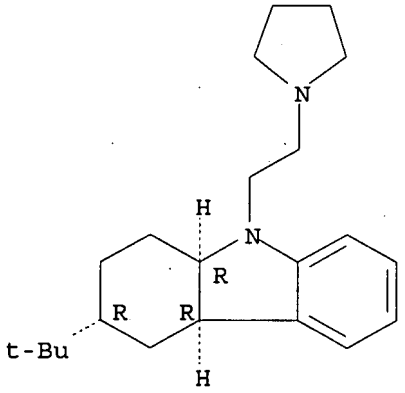


I

AB Tetrahydrocarbazoles I (R = Me, Et, CHMe2, CMe3, CH2CMe3; R1 = NMe2, NEt2, 1-pyrrolidinyl, 1-piperidyl) were prepared Some of them showed gastric secretion inhibitory properties. Structure activity relationships of I were studied.

IT 106583-49-7P 106583-67-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and gastric secretion inhibition of)
RN 106583-49-7 HCAPLUS
CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro-9-[2-(1-pyrrolidinyl)ethyl]-, monohydrochloride, (3α,4aα,9aα)-(9CI) (CA INDEX NAME)

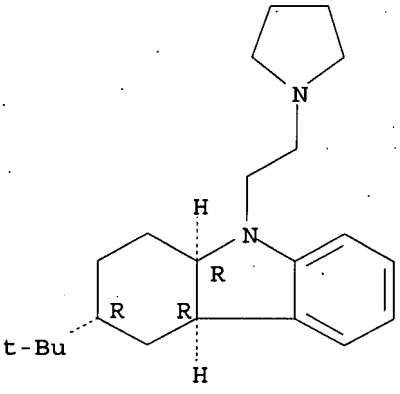
Relative stereochemistry.



● HCl

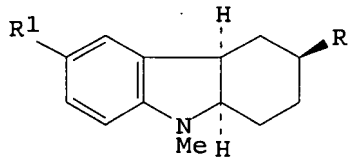
RN 106583-67-9 HCAPLUS
CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro-9-[2-(1-pyrrolidinyl)ethyl]-, (3α,4aα,9aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1979:22056 HCAPLUS
DOCUMENT NUMBER: 90:22056
TITLE: Substituent effects in saturated systems. An assessment of the transmission of substituent effects by the field, σ-inductive, and π-inductive

effects in 3- and 6-substituted hexahydrocarbazoles
AUTHOR(S): Utley, James H. P.; Yeboah, Samuel O.
CORPORATE SOURCE: Dep. Chem., Queen Mary Coll., London, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1978), (8), 766-70
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



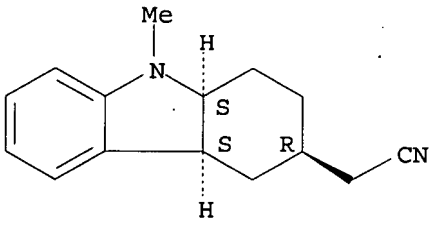
I

AB The basicities of the hexahydrocarbazoles I (R = H, Me, CH2OH, CH2OMe, CH2CN, R1 = H; R = H, R1 = Me, CMe2CN, CH2OH, CH2OMe, CH2CN) were measured. For substituents of the type CH2R2 polar effects are analyzed in terms of the direct field effect operating from the 3-position (R) and the field and π-inductive effect operating in concert across the aromatic portion of the mol. (from R1). Empirical correlations and the results of calcns. of ΔpKa using the Kirkwood-Westheimer method show that the field effect is substantial but that relay by the π-inductive effect is greater by a factor of .apprx.2.5.

IT 68384-50-9
RL: PRP (Properties)
(basicity of, transmission of substituent effect in relation to)

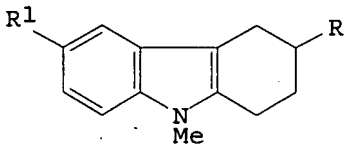
RN 68384-50-9 HCAPLUS
CN 1H-Carbazole-3-acetonitrile, 2,3,4,4a,9,9a-hexahydro-9-methyl-, (3α,4aβ,9aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:615158 HCAPLUS
DOCUMENT NUMBER: 89:215158
TITLE: Preparation of a series of 3- and 6-substituted 1,2,3,4-tetra- and 1,2,3,4,4a,9a-hexa-hydrocarbazoles
AUTHOR(S): Utley, James H. P.; Yeboah, Samuel O.
CORPORATE SOURCE: Dep. Chem., Queen Mary Coll., London, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1978), (8), 888-92

CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

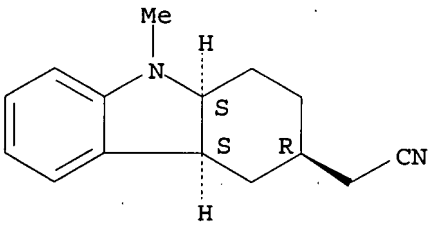
AB 4-Ethoxycarbonylcyclohexanone reacted with PhNMeNH2 in AcOH-HCl under reflux to give 30% tetrahydrocarbazole I (R = CO2H, R1 = H), which on reductive methylation (NaH-MeI-DMF) gave 60% I (R = CH2OMe, R1 = H) and on p-tolylsulfonylation gave 75% I (R = CH2O3SC6H4Me-4, R1 = H) (II). Treatment of II with NaCN-DMF gave 80% I (R = CH2CN, R1 = H) and II with pyridine.HCl-DMF gave 70% I (R = CH2Cl). Bischler reaction of 2-chlorocyclohexanone (III) with 4-H2NC6H4CO2Et followed by methylation gave 80% I (R = H, R1 = CO2Et), which on LiAlH4 reduction gave 70% I (R = H, R1 = CH2OH) (IV). Methylation of IV gave 50% I (R = H, R1 = CH2OMe). Bischler reaction of III with 4-H2NC6H4CH2CN gave 10% 6-cyanomethyl-1,2,3,4-tetrahydrocarbazole which on treatment with MeI gave 70% I (R = H, R1 = CMe2CN). Similarly, III with 4-MeNHC6H4CH2CN gave 20% I (R = H, R1 = CH2CN). Hydrogenation of I (R = CH2OH, CH2OMe, CH2CN, R1 = H; R = H, R1 = CO2Et, CH2OH, CH2OMe, CH2CN, CMe2CN) gave the corresponding syn,cis and cis-hexahydrocarbazoles, resp.

IT 68384-50-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 68384-50-9 HCAPLUS

CN 1H-Carbazole-3-acetonitrile, 2,3,4,4a,9,9a-hexahydro-9-methyl-, (3α,4aβ,9aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1971:448056 HCAPLUS
DOCUMENT NUMBER: 75:48056
TITLE: Substituent effects in saturated systems. Basicity, reactivity, and stereochemistry in 3- and 6-substituted cis-hexahydrocarbazoles
AUTHOR(S): Utley, J. H. P.; Smith, Alan
CORPORATE SOURCE: Queen Mary Coll., Univ. London, London, UK
SOURCE: Journal of the Chemical Society [Section] B: Physical Organic (1971), (6), 1201-7
CODEN: JCSPAC; ISSN: 0045-6470

DOCUMENT TYPE: Journal
LANGUAGE: English

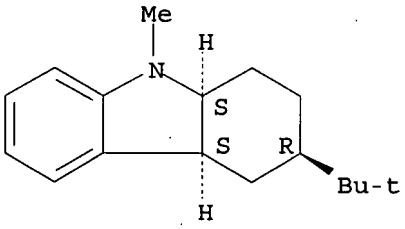
AB Rates of quaternization in MeCN and MeOH and pKa in H2O and aqueous BuO(CH2)2OH were determined for N-methyl-cis-1,2,3,4,4a,9a-hexahydrocarbazoles substituted (Me3C, Me, MeO) at the 3 and 6 positions. The decrease in basicity caused by 6-Me3C, syn-3-Me and syn-3-Me3C substitution is due to steric inhibition of general solvation of the conjugate acid, but this effect is offset by inhibition of H bonding to free base in the 3,3-di-Me derivative The differences in rates of quaternization accompanying a change of solvent are due to steric effects on H bonding involving the N lone pair and MeOH.

IT 25374-49-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(quaternization of, kinetics of)

RN 25374-49-6 HCAPLUS

CN Carbazole, 3β-tert-butyl-1,2,3,4,4aα,9aα-hexahydro-9-methyl- (8CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:465901 HCAPLUS
DOCUMENT NUMBER: 73:65901
TITLE: Conformation of syn- and anti-3-substituted cis-hexahydrocarbazoles from nuclear magnetic resonance coupling constants
AUTHOR(S): Shaw, Derek; Smith, Alan; Utley, J. H. P.
CORPORATE SOURCE: Dep. Chem., Queen Mary Coll., London, UK
SOURCE: Journal of the Chemical Society [Section] B: Physical Organic (1970), (6), 1161-5
CODEN: JCSPAC; ISSN: 0045-6470
DOCUMENT TYPE: Journal
LANGUAGE: English

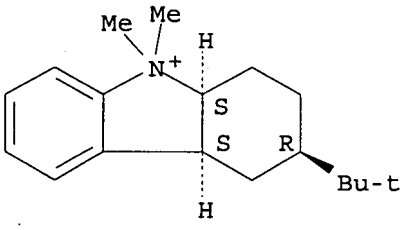
AB Double-irradiation expts. were used to interpret the NMR spectra of the methiodides of syn- and anti-3-substituted N-methyl-cis-hexahydrocarbazoles. The Karplus relation and conformational theory were used qual. to rationalize the characteristic splitting patterns and coupling consts. involving the ring junction protons, thus distinguishing between alternative conformations. For the syn series and the 3,3-dimethyl compound the alicyclic ring adopts a rigid shallow boat conformation. The anti compds. are probably conformationally mobile at probe temperature

IT 25374-59-8
RL: PRP (Properties)
(conformation of)

RN 25374-59-8 HCAPLUS

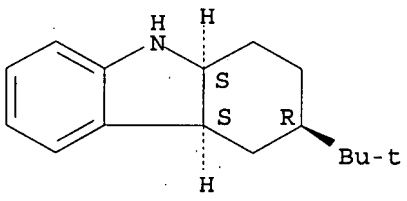
CN Carbazolium, 3β-tert-butyl-1,2,3,4,4aα,9aα-hexahydro-9,9-dimethyl-, iodide (8CI) (CA INDEX NAME)

Relative stereochemistry.



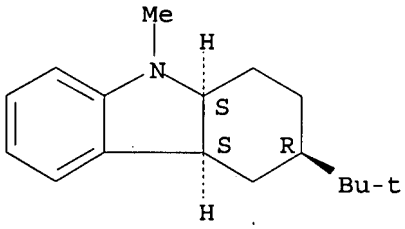
L25 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:55144 HCAPLUS
DOCUMENT NUMBER: 72:55144
TITLE: Configurational isomers of 3-substituted cis-hexahydrocarbazoles
AUTHOR(S): Smith, Alan; Utley, J. H. P.
CORPORATE SOURCE: Dep. Chem., Queen Mary Coll., London, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1970), (1), 1-5
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The preparation and properties of cis-hexahydrocarbazoles (I) substituted (tert-Bu, Me, and MeO) at the 3- and 6-positions are described. The role of protonation in the smooth catalytic hydrogenation of tetrahydrocarbazoles in ethanol-aqueous fluoroboric acid was confirmed. Configurational isomers, defined as syn and anti, were identified in the 3-substituted series o I; their configurations were assigned according to conformational theory and NMR spectroscopic data.
IT 25374-46-3P 25374-49-6P 25374-59-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 25374-46-3 HCAPLUS
CN Carbazole, 3β-tert-butyl-1,2,3,4,4aα,9aα-hexahydro- (8CI) (CA INDEX NAME)

Relative stereochemistry.



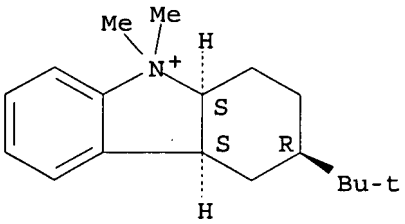
RN 25374-49-6 HCAPLUS
CN Carbazole, 3β-tert-butyl-1,2,3,4,4aα,9aα-hexahydro-9-methyl- (8CI) (CA INDEX NAME)

Relative stereochemistry.



RN 25374-59-8 HCAPLUS
CN Carbazolium, 3β-tert-butyl-1,2,3,4,4aα,9aα-hexahydro-9,9-dimethyl-, iodide (8CI) (CA INDEX NAME)

Relative stereochemistry.



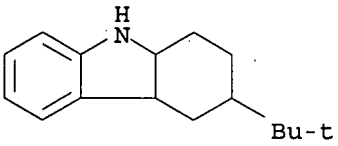
● I⁻

L25 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:35729 HCAPLUS
DOCUMENT NUMBER: 64:35729
ORIGINAL REFERENCE NO.: 64:6602a-b
TITLE: Some studies of the formation and structure of melanins
AUTHOR(S): Swan, George Albert
CORPORATE SOURCE: Univ. Newcastle-upon-Tyne, UK
SOURCE: Rend. Accad. Sci. Fis. Mat. (Soc. Nazl. Sci., Napoli) (1964), 31, 212-31
DOCUMENT TYPE: Journal
LANGUAGE: English

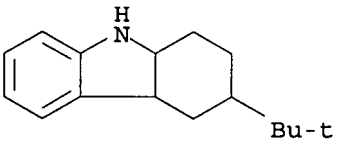
AB In addition to a literature review on the subject (25 references), studies are described of the formation of melanins (I), (a) enzymically, and (b) by autoxidn. from 2,3-(HO)2C6H3CH2CH(CO2H)NH2 (II) and 2,3-(HO)2C6H3CH2CH2NH2 (III). When II and III were labeled with D in the α or β position of the side chain and then converted to I, large retention of D was observed in the I. This suggests that the I are not polymers composed entirely of indole-5,6-quinone, but that they also contain uncyclized units of the precursors (or quinones derived from these) or (more probably) units of 2,3-dihydroindole-5,6-quinone. When I prepared from II-carboxy-14C was oxidized, the resulting pyrrole-2,3,5-tricarboxylic acid was radioactive while the pyrrole-2,3-dicarboxylic acid was inactive.

IT 6731-89-1
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 6731-89-1 HCAPLUS
CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA

INDEX NAME)



L25 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:35728 HCAPLUS
DOCUMENT NUMBER: 64:35728
ORIGINAL REFERENCE NO.: 64:6601g-h,6602a
TITLE: Catalytic hydrogenation of indoles
AUTHOR(S): Smith, A.; Utley, J. H. P.
CORPORATE SOURCE: Queen Mary Coll., London
SOURCE: Chemical Communications (London) (1965), (18), 427-8
CODEN: CCOMA8; ISSN: 0009-241X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 64:35728
GI For diagram(s), see printed CA Issue.
AB Indoles (I), 1 g., were hydrogenated in EtOHHBF4 solution over 0.01-0.5 g. PtO2 at 1 atmospheric and room temperature to give quant. the corresponding indolines (R1, R2, and m.p. or b.p./mm. given): H, H, m. 95-6°; Me, H, m. 30-1°, H, Me, m. 54-6°; tert-Bu, H, m. 64-5°; H, tert-Bu, m. 75-7°.
IT 6731-89-1P, Carbazole, 3-tert-butyl-1,2,3,4,4a,9a-hexahydro-
RL: PREP (Preparation)
(formation in 3-tert-butyl-1,2,3,4-tetrahydrocarbazole hydrogenation)
RN 6731-89-1 HCAPLUS
CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)



L25 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1952:57425 HCAPLUS
DOCUMENT NUMBER: 46:57425
ORIGINAL REFERENCE NO.: 46:9616h-i,9617a-e
TITLE: Imidazolines
INVENTOR(S): Hartman, Max; Studer, Siegfried
PATENT ASSIGNEE(S): C I B A Pharmaceutical Products, Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

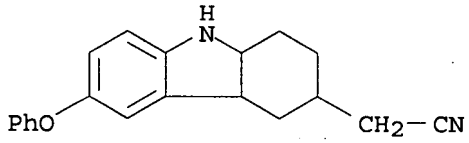
US 2569415 19510925 US 1948-65067 19481213

AB 2-(9-Carbazolylalkyl)imidazolines (I) and their salts of inorg. or organic acids are prepared by treating a 9-carbazolealkanecarboxylic acid or its reactive acid derivative with a N-unsubstituted alkylenediamine or its reactive N-derivative I and their salts exhibit an action similar to that of adrenaline. 9-Carbazoleacetic acid 45 and (CH2NH2)2.H2O 16 in warm alc. 300 parts by weight is mixed with 1 equivalent HCl in EtOH, the whole heated to about 230°, the EtOH distilled off, the mixture stirred 0.5 h., 28.4 parts P2O5 added, the temperature kept 1.5 h. at 230°, and the mass cooled, pulverized, and extracted with hot H2O; the filtered solution yields 2-(9-carbazolylmethyl)-2-imidazoline, m. 232-234° (from EtOH). (HCl salt, m. 270-2°). Et 1,2,3,4,-tetrahydro-9-carbazoleacetate yields 2-(1,2,3,4-tetrahydro-9-carbazolylmethyl)-2-imidazoline, m. 180-1°; HCl salt, decompose 275-7.5°. 9-(Cyanomethyl)-1,2,8,4-tetrahydrocarbazole yields 2-(1,2,3,4-tetrahydro-9-carbazolylmethyl)-2-imidazoline, m. 132-3°, (HCl salt, m. 210-11° (decomposition). 9-(2-Cyanoethyl)carbazole produces 2-[2-(9-carbazolyl)ethyl]-2-imidazoline (HCl salt, m. 253°). 2-[2-(1,2,3,4-Tetrahydro-9-carbazolyl)ethyl]-2-imidazoline (HCl salt, m. 213-15°), is prepared from 9-(2-cyanoethyl)tetrahydrocarbazole. 2-Chlorocyclohexanone condensed with anilines substituted in the 4-position yields the 5,6,7,8-tetrahydrocarbazoles (II) substituted in the 3-position; the 3-PhO compound b0.1 209-10°, m. 141-3°. The II by reduction with Sn and concentrated HCl in EtOH yield the corresponding carbazolines: 3-Me, b0.5 114-15°; 3-MeO, b0.4 128-9°; 3-EtO, b0.18 132-4°; 3-PhO, b0.2 196-8°; 3-Cl, b0.38 134°, m. 62-4°. By treating the above carbazolines with trioxymethylene and aqueous KCN solution in glacial AcOH at 5-10° and then stirring 20 h. at room temperature may be prepared the following 9-(cyanomethyl)carbazolines: 3-Me, b0.32 157-8°; 3-MeO, m. 107-8°; 3-EtO, m. 102.5-3.5°; 3-PhO, m. 119.5-20.5°; 3-Cl, m. 81-2°. Upon dehydrogenation with chloranil in boiling xylene, the substituted 9-(cyanomethyl)carbazolines are converted into the corresponding 9-(cyanomethyl)carbazoles. 3-Methoxy-9-(cyanomethyl)carbazole (III), m. 116-17°, 17 refluxed 1 h. at a bath temperature of 220° with p-MeC6H4SO3NH3CH2CH2NH2 16.3 parts, the crystalline product dissolved in dilute EtOH, the solution made alkaline to phenolphthalein with 5 N NaOH, the precipitated crystalline powder dissolved in CH2Cl2, the solution dried over KOH and the CH2Cl2 evaporated gives 91.3% 2-(3-methoxy-9-carbazolylmethyl)-2-imidazoline (IV), m. 182-3° (after distillation in a high vacuum and recrystn. from EtOH); HCl salt, m. 227-8°. Similarly, the following analogs of III yield the corresponding analogs of IV. 3-Me analog of III, 9-(cyanomethyl)carbazole, m. 141-2°; of IV, m. 171-2.5° (HCl salt, m. 271-3°). 3-EtO analog of III, m. 95-7°; of IV, m. 164-5° (HCl salt, m. 242-2.5°). 3-PhO analog of III, m. 105-6°; of IV, m. 172.5-3.5° (HCl salt, m. 271-2°). 3-Cl analog of III; of IV, m. 213-15° (HCl salt, m. 263-5°).

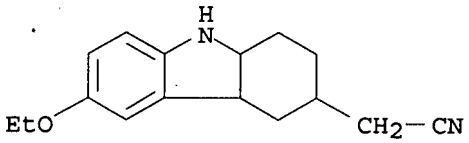
IT 854825-67-5P, 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-phenoxy- 854825-68-6P, 9-Carbazoleacetonitrile, 6-ethoxy-1,2,3,4,4a,9a-hexahydro- 854825-69-7P, 9-Carbazoleacetonitrile, 6-chloro-1,2,3,4,4a,9a-hexahydro- 855712-17-3P, 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-methoxy- 855712-19-5P, 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-methyl-
RL: PREP (Preparation)
(preparation of)

RN 854825-67-5 HCAPLUS

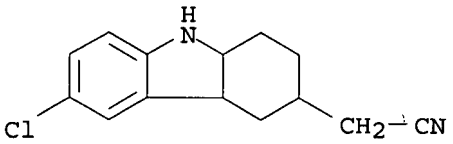
CN 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-phenoxy- (5CI) (CA INDEX NAME)



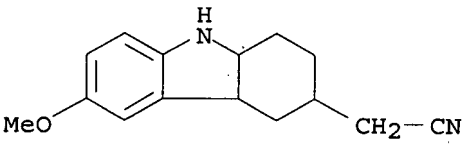
RN 854825-68-6 HCAPLUS
CN 9-Carbazoleacetonitrile, 6-ethoxy-1,2,3,4,4a,9a-hexahydro- (5CI) (CA INDEX NAME)



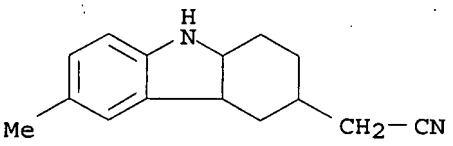
RN 854825-69-7 HCAPLUS
CN 9-Carbazoleacetonitrile, 6-chloro-1,2,3,4,4a,9a-hexahydro- (5CI) (CA INDEX NAME)



RN 855712-17-3 HCAPLUS
CN 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-methoxy- (5CI) (CA INDEX NAME)



RN 855712-19-5 HCAPLUS
CN 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-methyl- (5CI) (CA INDEX NAME)



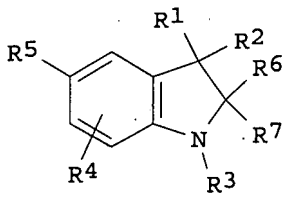
=> d l34 ibib abs hitstr tot

L34 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:790472 HCAPLUS
DOCUMENT NUMBER: 133:335158
TITLE: Preparation of 3,3-substituted indolines as progesterone receptor antagonists
INVENTOR(S): Ullrich, John W.; Fensome, Andrew; Zhi, Lin; Jones, Todd K.; Marschke, Keith B.; Tegley, Christopher M.
PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066554	A1	20001109	WO 2000-US11464	20000501 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6417214	B1	20020709	US 2000-552352	20000419 <--
CA 2371629	A1	20001109	CA 2000-2371629	20000501 <--
EP 1175397	A1	20020130	EP 2000-930201	20000501 <--
EP 1175397	B1	20040818		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002543181	T	20021217	JP 2000-615385	20000501 <--
AT 273951	T	20040915	AT 2000-930201	20000501
PT 1175397	T	20050131	PT 2000-930201	20000501
ES 2226838	T3	20050401	ES 2000-930201	20000501
US 2003008909	A1	20030109	US 2002-131379	20020424 <--
US 6835744	B2	20041228		
HK 1043986	A1	20050401	HK 2002-104852	20020628

PRIORITY APPLN. INFO.:		
US 1999-183061P	P	19990504
US 2000-552352	A1	20000419
WO 2000-US11464	W	20000501

OTHER SOURCE(S): MARPAT 133:335158
GI



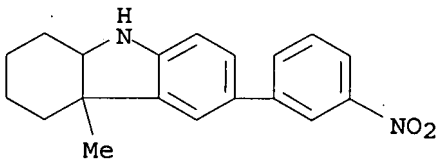
I

AB The title compds. [I; R1, R2 = H, OH, OAc, etc.; or R1 and R2 are joined to form a ring comprising CH2(CH2)nCH2, CH2CH2CMe2CH2CH2, O(CH2)mCH2, etc.; or R1 and R2 together comprise a double bond to CMe2, C(cycloalkyl), O, C(cycloether); n = 0-5; m = 1-4; R3 = H, OH, NH2, etc.; R4 = H, halo, CN, etc.; R5 = optionally substituted Ph, a 5-6 membered heterocycle, a 4- or 7-substituted indole, substituted benzothiophene; R6, R7 = H, Me, Et, etc.] which are progesterone receptor antagonists, and are useful in inducing contraception, and treating or preventing benign or malignant neoplastic disease, were prepared Thus reacting 5-bromo-2,3,3-trimethyl-2,3-dihydro-1H-indole (preparation given) with 3-nitrophenylboronic acid in the presence of Pd(PPh3)4 afforded 82% I [R1, R2 = Me; R3, R4 = H; R5 = 3-O2NC6H4; R6 = Me; R7 = H]. In general, compds. I were effective at 0.5-500 mg/kg/day.

IT 304468-33-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3,3-substituted indolines as progesterone receptor antagonists)

RN 304468-33-5 HCAPLUS

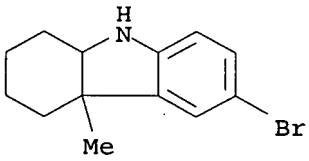
CN 1H-Carbazole, 2,3,4,4a,9,9a-hexahydro-4a-methyl-6-(3-nitrophenyl)- (9CI) (CA INDEX NAME)



IT 304468-40-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3,3-substituted indolines as progesterone receptor antagonists)

RN 304468-40-4 HCAPLUS

CN 1H-Carbazole, 6-bromo-2,3,4,4a,9,9a-hexahydro-4a-methyl- (9CI) (CA INDEX NAME)



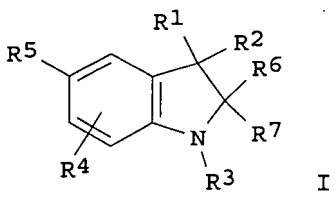
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:790349 HCAPLUS
DOCUMENT NUMBER: 133:350134
TITLE: Preparation of 3,3-substituted indolines useful in contraceptive compositions
INVENTOR(S): Grubb, Gary S.; Zhi, Lin; Jones, Todd K.; Tegley, Christopher M.; Ullrich, John W.; Fensome, Andrew; Wrobel, Jay E.; Edwards, James P.
PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066166	A1	20001109	WO 2000-US11748	20000501 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6329416	B1	20011211	US 2000-552631	20000419 <--
CA 2372591	A1	20001109	CA 2000-2372591	20000501 <--
EP 1173211	A1	20020123	EP 2000-928667	20000501 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002543157	T	20021217	JP 2000-615050	20000501 <--
US 2002035099	A1	20020321	US 2001-977790	20011015 <--
US 6503939	B2	20030107		

PRIORITY APPLN. INFO.:
US 1999-183057P P 19990504
US 2000-552631 A1 20000419
WO 2000-US11748 W 20000501

OTHER SOURCE(S): MARPAT 133:350134
GI



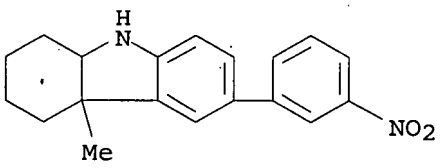
I

AB The title compds. [I; R1, R2 = H, OH, OAc, etc.; or R1 and R2 are joined to form a ring comprising CH2(CH2)nCH2, CH2CH2CMe2CH2CH2, O(CH2)mCH2, etc.; or R1 and R2 together comprise a double bond to CMe2, C(cycloalkyl), O, C(cycloether); n = 0-5; m = 1-4; R3 = H, OH, NH2, etc.; R4 = H, halo, CN, etc.; R5 = optionally substituted Ph, a 5-6 membered heterocycle, a 4- or 7-substituted indole, substituted benzothiophene; R6, R7 = H, Me, Et, etc.] which are progesterone receptor antagonists, and are useful in inducing contraception, and treating or preventing benign or malignant neoplastic disease, were prepared Thus reacting 5-bromo-2,3,3-trimethyl-2,3-dihydro-1H-indole (preparation given) with 3-nitrophenylboronic acid in the presence of Pd(PPh3)4 afforded 82% I [R1, R2 = Me; R3, R4 = H; R5 = 3-O2NC6H4; R6 = Me; R7 = H]. In general, compds. I were effective at 0.5-500 mg/kg/day..

IT 304468-33-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3,3-substituted indolines as progesterone receptor antagonists)

RN 304468-33-5 HCAPLUS

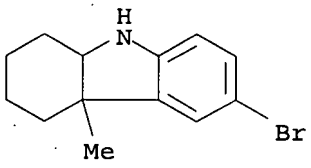
CN 1H-Carbazole, 2,3,4,4a,9,9a-hexahydro-4a-methyl-6-(3-nitrophenyl)- (9CI) (CA INDEX NAME)



IT 304468-40-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3,3-substituted indolines as progesterone receptor antagonists)

RN 304468-40-4 HCAPLUS

CN 1H-Carbazole, 6-bromo-2,3,4,4a,9,9a-hexahydro-4a-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:787188 HCAPLUS
DOCUMENT NUMBER: 123:198832
TITLE: Tetracyclic condensed heterocyclic compounds for the treatment of senile dementia.
INVENTOR(S): Goto, Giichi; Ishihara, Yuji; Miyamoto, Masaomi
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

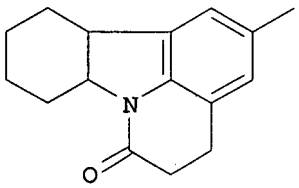
SOURCE: Eur. Pat. Appl., 53 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

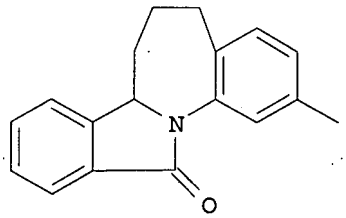
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 655451	A1	19950531	EP 1994-118734	19941129 <--
EP 655451	B1	20010620		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
US 5620973	A	19970415	US 1994-330133	19941025 <--
CA 2136913	A1	19950531	CA 1994-2136913	19941129 <--
JP 07309835	A	19951128	JP 1994-294754	19941129 <--
AT 202354	T	20010715	AT 1994-118734	19941129 <--
US 5814642	A	19980929	US 1996-681911	19960730 <--

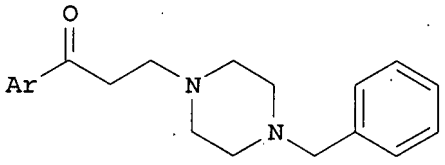
PRIORITY APPLN. INFO.: JP 1993-299799 A 19931130
JP 1994-55984 A 19940325
US 1994-330133 A3 19941025

OTHER SOURCE(S): CASREACT 123:198832; MARPAT 123:198832

GI

Q1= 

Q2= 

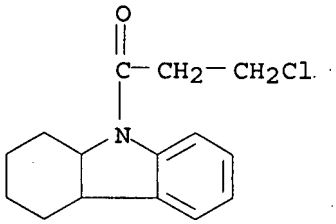


I

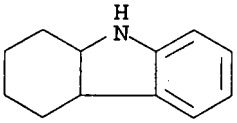
AB Title compds. ArCO(CHR1)nY [Ar = (un)substituted tetracyclic fused heterocyclic group; R1 = H or (un)substituted hydrocarbyl; n = 1-10; Y = amino or N-containing saturated (un)substituted heterocyclic group] and their salts are claimed. The compds. show excellent cholinesterase inhibitory activity and monoamine uptake inhibitory activity, thus being useful as therapeutic and/or prophylactic medicaments for senile dementia and Alzheimer's disease, and also as antidepressants. For example, 1,2,3,4,4a,9a-hexahydrocarbazole underwent N-acylation by ClCH2CH2COCl, Friedel-Crafts cyclization by AlCl3, and Friedel-Crafts acylation by treatment with both ClCH2CH2COCl and AlCl3, to give pyridocarbazolone derivative ArCOCH2CH2Cl [Ar = Q1]. Reaction of the latter with 1-benzylpiperazine gave title compound I [Ar = Q1] as the di-HCl salt. The similarly prepared compound I [Ar = Q2] had IC50 of 0.0164 μM for inhibition of rat cerebral cholinesterase in vitro, vs. 0.220 for physostigmine and 0.300 for THA. The same compound was also as potent as imipramine in a monoamine uptake inhibitor assay.

IT 167633-68-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(intermediate; preparation of tetracyclic heterocyclics for treatment of senile dementia)
RN 167633-68-3 HCAPLUS
CN 1H-Carbazole, 9-(3-chloro-1-oxopropyl)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)



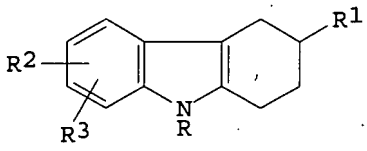
IT 1775-86-6, 1,2,3,4,4a,9a-Hexahydrocarbazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of tetracyclic heterocyclics for treatment of senile dementia)
RN 1775-86-6 HCAPLUS
CN 1H-Carbazole, 2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)



L34 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:47136 HCAPLUS
DOCUMENT NUMBER: 94:47136
TITLE: Tetrahydrocarbazoles and pharmaceutical compositions for treating heart failure in mammals
INVENTOR(S): Mooradian, Aram
PATENT ASSIGNEE(S): Sterling Drug Inc., USA
SOURCE: U.S., 7 pp. Cont.-in-part of U.S. Ser. No. 465,238, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
US 4224335	A	19800923	US 1976-651882		19760123	<--
US 3642816	A	19720215	US 1967-659606		19670810	<--
US 3959309	A	19760525	US 1973-425205		19731217	<--
PRIORITY APPLN. INFO.:			US 1967-659606	A2	19670810	
			US 1969-793545	A2	19690123	
			US 1971-172206	A2	19710816	
			US 1973-425205	A2	19731217	
			US 1974-465238	A2	19740429	
			CA 1968-10686	A	19680124	

OTHER SOURCE(S): MARPAT 94:47136
GI

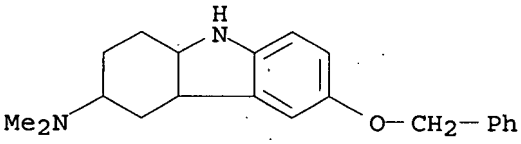


I

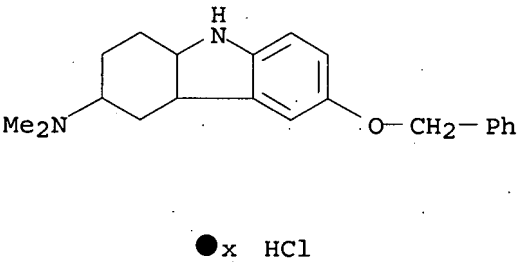
AB The carbazoles I (R = H, Me; R1 = NH2, EtNH, Me2N; R2 = 5-, 6-, 7-HO; R3 = H, 7-F, 7-HO) were prepared Thus, m-PhCH2OC6H4NMeNH2.HCl was cyclized with 4-(dimethylamino)cyclohexanone to give I (R = Me, R1 = Me2N, R2 = 7-PhCH2O, R3 = H), which was debenzylated to give I (R = Me, R1 = Me2N, R2 = 7-HO, R3 = H). I underwent cardiotonic tests and were found useful for treatment of congestive heart failure in mammals.

IT 76243-30-6 76243-31-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(debenzylation of)

RN 76243-30-6 HCAPLUS
CN 1H-Carbazol-3-amine, 2,3,4,4a,9,9a-hexahydro-N,N-dimethyl-6-(phenylmethoxy)- (9CI) (CA INDEX NAME)

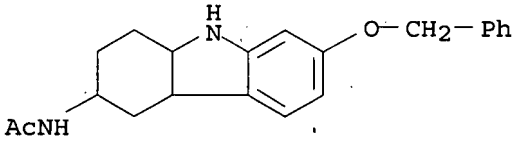


RN 76243-31-7 HCAPLUS
CN 1H-Carbazol-3-amine, 2,3,4,4a,9,9a-hexahydro-N,N-dimethyl-6-(phenylmethoxy)-, hydrochloride (9CI) (CA INDEX NAME)

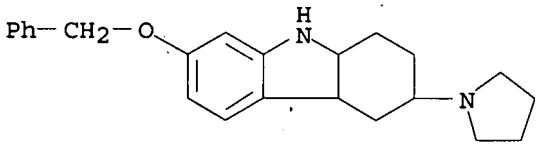


IT 76243-19-1P 76243-22-6P 76243-27-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and debenzylation of)

RN 76243-19-1 HCAPLUS
CN Acetamide, N-[2,3,4,4a,9,9a-hexahydro-7-(phenylmethoxy)-1H-carbazol-3-yl]- (9CI) (CA INDEX NAME)

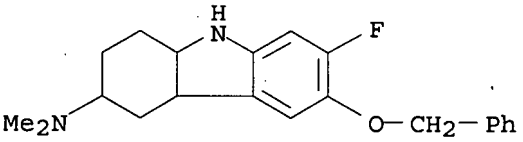


RN 76243-22-6 HCAPLUS
CN 1H-Carbazole, 2,3,4,4a,9,9a-hexahydro-7-(phenylmethoxy)-3-(1-pyrrolidinyl)-, hydrochloride (9CI) (CA INDEX NAME)



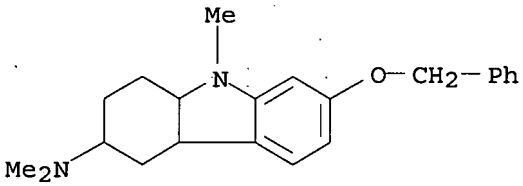
●x HCl

RN 76243-27-1 HCAPLUS
CN 1H-Carbazol-3-amine, 7-fluoro-2,3,4,4a,9,9a-hexahydro-N,N-dimethyl-6-(phenylmethoxy)-, hydrochloride (9CI) (CA INDEX NAME)



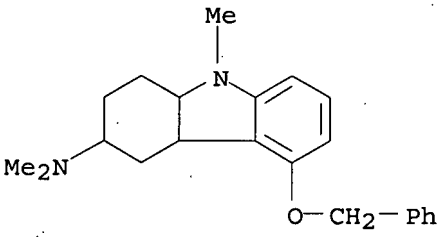
●x HCl

IT 76243-05-5P 76243-06-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
RN 76243-05-5 HCAPLUS
CN 1H-Carbazol-3-amine, 2,3,4,4a,9,9a-hexahydro-N,N,9-trimethyl-7-(phenylmethoxy)-, hydrochloride (9CI) (CA INDEX NAME)



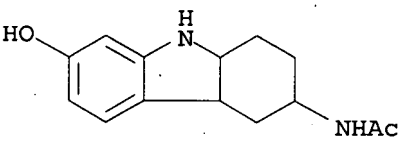
●x HCl

RN 76243-06-6 HCAPLUS
CN 1H-Carbazol-3-amine, 2,3,4,4a,9,9a-hexahydro-N,N,9-trimethyl-5-(phenylmethoxy)-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

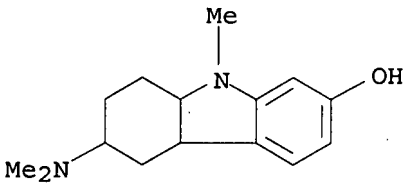
IT 76243-20-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 76243-20-4 HCAPLUS
CN Acetamide, N-(2,3,4,4a,9,9a-hexahydro-7-hydroxy-1H-carbazol-3-yl)- (9CI) (CA INDEX NAME)



IT 76243-10-2P 76243-14-6P 76243-32-8P
76254-53-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 76243-10-2 HCAPLUS
CN 1H-Carbazol-7-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-9-methyl-, methanesulfonate (salt) (9CI) (CA INDEX NAME)

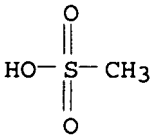
CM 1

CRN 76243-09-9
CMF C15 H22 N2 O

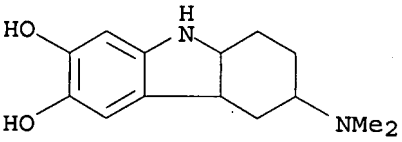


CM 2

CRN 75-75-2
CMF C H4 O3 S



RN 76243-14-6 HCAPLUS
CN 1H-Carbazole-6,7-diol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-, hydrobromide (9CI) (CA INDEX NAME)

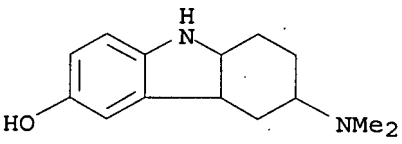


●x HBr

RN 76243-32-8 HCAPLUS
CN 1H-Carbazol-6-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

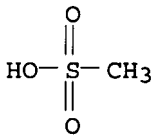
CM 1

CRN 76243-03-3
CMF C14 H20 N2 O

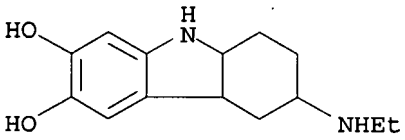


CM 2

CRN 75-75-2
CMF C H4 O3 S

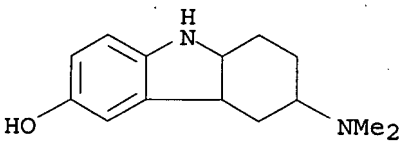


RN 76254-53-0 HCAPLUS
CN 1H-Carbazole-6,7-diol, 3-(ethylamino)-2,3,4,4a,9,9a-hexahydro-, hydrobromide (9CI) (CA INDEX NAME)

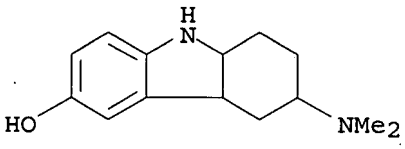


●x HBr

IT 76243-03-3P 76243-04-4P 76243-07-7P
76243-08-8P 76243-13-5P 76243-17-9P
76243-18-0P 76243-21-5P 76243-23-7P
76243-29-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for treatment of congestive heart failure)
RN 76243-03-3 HCAPLUS
CN 1H-Carbazol-6-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)

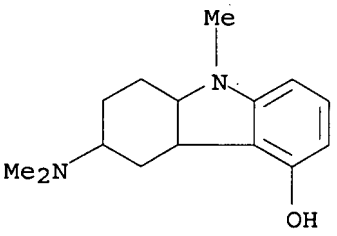


RN 76243-04-4 HCAPLUS
CN 1H-Carbazol-6-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-, hydrochloride (9CI) (CA INDEX NAME)



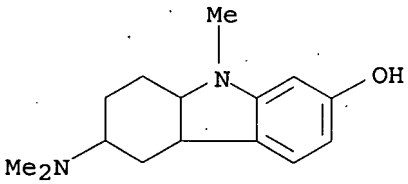
● x HCl

RN 76243-07-7 HCAPLUS
CN 1H-Carbazol-5-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-9-methyl-, hydrochloride (9CI) (CA INDEX NAME)



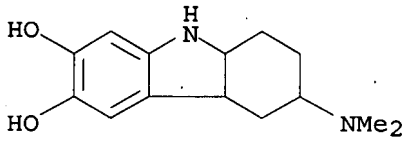
● x HCl

RN 76243-08-8 HCAPLUS
CN 1H-Carbazol-7-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-9-methyl-, hydrochloride (9CI) (CA INDEX NAME)



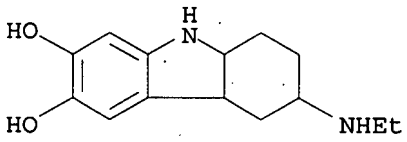
● x HCl

RN 76243-13-5 HCAPLUS
CN 1H-Carbazole-6,7-diol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-, hydrochloride (9CI) (CA INDEX NAME)



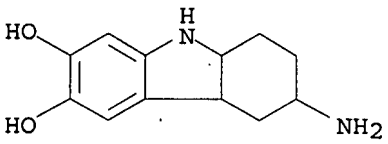
●x HCl

RN 76243-17-9 HCAPLUS
CN 1H-Carbazole-6,7-diol, 3-(ethylamino)-2,3,4,4a,9,9a-hexahydro-, hydrochloride (9CI) (CA INDEX NAME)



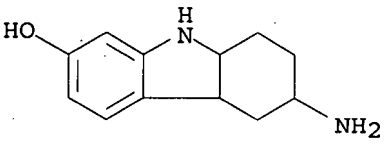
●x HCl

RN 76243-18-0 HCAPLUS
CN 1H-Carbazole-6,7-diol, 3-amino-2,3,4,4a,9,9a-hexahydro-, hydrochloride (9CI) (CA INDEX NAME)



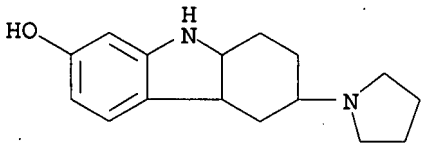
●x HCl

RN 76243-21-5 HCAPLUS
CN 1H-Carbazol-7-ol, 3-amino-2,3,4,4a,9,9a-hexahydro-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

RN 76243-23-7 HCAPLUS
CN 1H-Carbazol-7-ol, 2,3,4,4a,9,9a-hexahydro-3-(1-pyrrolidinyl)-, hydrochloride (9CI) (CA INDEX NAME)

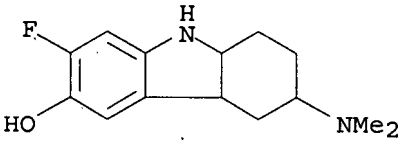


● x HCl

RN 76243-29-3 HCAPLUS
CN 1H-Carbazol-6-ol, 3-(dimethylamino)-7-fluoro-2,3,4,4a,9,9a-hexahydro-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

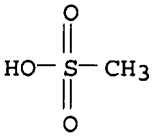
CM 1

CRN 76243-28-2
CMF C14 H19 F N2 O



CM 2

CRN 75-75-2
CMF C H4 O3 S



=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	120.93	1505.14

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-14.82	-14.82

STN INTERNATIONAL LOGOFF AT 14:37:48 ON 10 AUG 2007